

SYMPOSIUM ON PYROLYSIS PRODUCTS DERIVED FROM COAL,
OIL SHALE, TAR SANDS, BIOMASS, AND HEAVY OIL

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STATUS OF THE CHARACTERIZATION OF JET
FUELS FROM COAL LIQUIDS

by

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INTRODUCTION

In the future, jet fuels will need higher densities and higher heat contents. These fuels will increase the range of aircraft and/or permit heavier payloads to be transported. Furthermore, these fuels will also be required to function as heat exchange fluids to remove heat from leading edges and vital engine parts. Very stringent specifications are placed on the composition, physical and chemical properties, thermal stability, and stability upon storage of fuels for commercial and military jet engines. Of the three basic hydrocarbon types -- paraffins, naphthenes (cycloparaffins), and aromatics -- naphthenes have the most desirable properties for jet fuels. One potential source of such a fuel is coal. Many of the compounds in coal are aromatic, and coal liquefaction products are likewise highly aromatic. Coal liquids can be further hydrotreated to produce naphthenes.

Many studies have involved the production of conventional and high-density jet fuels from coal liquids [1-21]. Sullivan et al., at Chevron Research Company, Richmond, California, conducted a number of studies for the Department of Energy to assess the feasibility of refining synthetic coal liquid feedstocks to distillate fuels, such as high-density jet fuels [5-14,22-24]. The upgrading of products from single-stage processes, such as SRC-II [5,8], H-Coal [6,8,14], and EDS [7-8], and from two-stage coal liquefaction processes, such as the Lummus Crest Integrated Two-Stage Liquefaction Process (ITSL) [9-11,13-14] and the HRI Catalytic Two-Stage Liquefaction Process (CTSL) [12-14], has been carried out. "Key factors that determine how easy or difficult a particular syncrude is to refine are EP [endpoint], boiling range, hydrogen content, and heteroatom content [14]."

In September 1986, the Fuels Branch of the Aero Propulsion Laboratory at Wright-Patterson Air Force Base, Ohio, began an investigation of the potential for production of jet fuel from the liquid by-product streams produced by the gasification of lignite at the Great Plains Gasification Plant located in Beulah, North Dakota. Funding was provided to the Department of Energy (DOE) from the Air

Force to administer the experimental portion of the effort. The Morgantown Energy Technology Center administered the effort (DOE Contract Number DE-FC21-86MC11076) at Western Research Institute, which studied the potential of the liquid by-product streams for the production of jet fuels [25]. The Pittsburgh Energy Technology Center (PETC) administered the effort (DOE Contract Number DE-AC22-87PC90016) at the University of North Dakota Energy and Mineral Research Center, which characterized these liquid by-product streams [26]. The PETC also administered the effort (DOE Contract Number DE-AC22-87PC90015) of Amoco Oil Company and Lummus Crest, which conducted a preliminary analysis of upgrading alternatives for the production of aviation turbine fuels from the Great Plains liquid product streams [27]. A small research effort was also conducted in-house at PETC.

The in-house research effort at PETC sought to further characterize jet fuels produced at Chevron and the coal-derived syncrudes from which they were prepared. While some of the characterization data may replicate the work of Sullivan et al. [9,10,12,22-24], the nuclear magnetic resonance data (NMR), the low-voltage high-resolution mass spectrometric (LVHRMS) data, and the test of "fit" to correlations previously developed at PETC for narrow-boiling range coal distillates are supplemental to and amplify the characterizations performed at Chevron. Furthermore, in-house characterization of the properties of the Great Plains tar oil was carried out, including NMR and LVHRMS analyses. The tar oil was distilled and the bottoms were hydrotreated. The overhead and bottoms (before and after hydro-treatment) were similarly characterized.

Interest in the properties of these materials and of similar materials derived from tar sands and oil shale culminated in a symposium on the structure of future jet fuels presented before the Division of Petroleum Chemistry at the American Chemical Society Meeting in Denver, April 5-10, 1987. At that symposium, Sullivan gave a summary report on this investigation related to high-density fuels from coal [24]. It was also at that meeting that Knudson et al. presented results of their evaluation of jet fuels from tar oil obtained from the Great Plains Gasification Plant (GPGP) at Beulah, North Dakota [28].

The present report will compare results of analyses and correlations of properties carried out on samples of high-density fuels from the ITSL process. These samples were produced at Chevron. We will also describe in part those investigations carried out on GPGP tar oil.

EXPERIMENTAL

Samples that have been characterized at the PETC from the ITSL process include three wide-boiling-range coal-derived syncrudes and four jet-boiling-range products produced at Chevron. The syncrudes include an Illinois No. 6 coal-derived oil, and a light and heavy oil derived from Wyodak. The jet-boiling-range products include hydrotreated Wyodak light and heavy oils, and hydrotreated and hydrocracked Illinois No. 6 oils. Procedures used for upgrading the syncrudes have been reported [9-10]. Other samples that have been characterized include the GPGP tar oil stream, as well as the overhead and bottoms from distillation of the tar oil and the hydrotreated distillation bottoms of the tar oil; the North Dakota lignite used to produce the tar was also characterized.

Chemical and physical property measurements were carried out at PETC and at Huffman Laboratories (Wheatridge, Colorado); and numerous property measurements were reported by Sullivan [9-10,12,22-24]. Characterizations include simulated

distillation by gas chromatography (ASTM D2887) for boiling-point-range determination [29], CHONS elemental analysis [30-32], Karl Fischer determination of water [33], molecular weight [32], refractive index [34], specific gravity [32], viscosity [35], Carbon-13 and proton NMR [36], IR [37], low-resolution mass spectrometry with an ionizing voltage of 70 eV (ASTM D2789 type analysis was used to calculate the compound classes), and LVHRMS [38-39]. Detailed results of these analyses are the subject of an in-house report in preparation [40]. The data relevant to this report are summarized in Tables 1 through 6. Additionally, correlations developed at PETC for narrow-boiling-range coal liquid distillates [41] were applied to these samples.

The Great Plains Gasification Plant operated by the ANG Coal Gasification Company for the Department of Energy produces 150 million scf of substitute natural gas per day [26]. Three by-product hydrocarbon liquid streams -- tar oils, crude phenols, and naphtha -- are also produced. Of the three liquid streams, the tar oil stream (produced at the rate of 2900 bbl/day [27]) is thought the most appropriate for conversion to jet fuel [26]. The tar oil from the GPGP had a boiling range of 107°C to 524°C. About 20 liters of the tar oil were vacuum distilled to an atmospheric equivalent cut point of 350°C at the University of Pittsburgh Applied Research Center. About 66% of the tar oil was found in the overhead, and 34% in the vacuum bottoms. A 300-g portion of the 350°C+ bottoms was hydrotreated in a 1-liter batch autoclave at 350°C under 13.6 MPa H₂ (3 scf/hr) using a presulfided Shell 324 catalyst for one hour. Five runs were made and a total of 1500 g of product hydrotreated.

RESULTS AND DISCUSSION

Coal liquids derived from two-stage processes were lower in oxygen and nitrogen, and for a given boiling range, Sullivan found these liquids easier to upgrade than products from single-stage processes [14]. The properties of jet-fuel products, consisting mostly of cyclic hydrocarbons, were virtually the same from both the single-stage and two-stage processes. For all processes evaluated at Chevron, the jet-fuel products had high densities and high volumetric energy contents. The Wyodak CTSI light oil [12] was easier to upgrade than the other syncrudes, apparently because of its low-boiling-point end point, higher hydrogen content, and lower heteroatom content [14]. For syncrudes with a high-boiling-point end point, a successful upgrading procedure was developed that consisted of a two-step process: (1) hydrotreatment for heteroatom removal and (2) low-temperature hydrogenation for aromatic saturation [9,13,14].

The hydrotreatment process that produces the jet-boiling-range products from the coal-derived syncrudes removes heteroatoms, breaks down heavy paraffins into lighter paraffins, and hydrogenates aromatic rings, creating cyclic aliphatic functionalities. This is observed in the characterization data. The hydrogen contents of the hydrotreated products are greater than those of the syncrudes; and proton NMR, as well as carbon-13 NMR, confirms the predominance of aliphatics over aromatics in the hydrotreated product versus the predominance of aromatics in the syncrude. Results from LVHRMS and low-resolution mass spectrometry indicate a larger amount of the desirable lighter cyclic hydrocarbons in the jet-boiling-range products than in the corresponding syncrudes.

Table 3 compares properties of the four jet-fuel products prepared and characterized by Sullivan [9,10,12], and further characterized and studied here, to those of a Jet A specification fuel [13] and a high-density fuel [42]. The coal-derived jet-fuel products meet most of the Jet A and high-density fuel speci-

cations. The Illinois ITSL hydrocracked product exceeds the minimum for flash point, and the distribution of hydrocarbon types does not quite meet the specifications, although a high concentration of naphthenes is desirable. The four jet-fuel products do exceed the API gravity specifications, that is, they have higher densities than the specification fuels. This specification, however, is probably not necessary for aircraft with modern fuel-flow controllers [14]. There were previously no jet-fuel products with an API gravity below 37 that have met the other specifications [13]. The higher densities would probably be an advantage, since the fuel would have a higher volumetric energy content. These four products otherwise meet most of the jet-fuel specifications and have the desirable high naphthenic content and thus have potential for serious consideration as aviation jet fuels.

Franck et al. [43] recently concluded that two- or three-ring cycloparaffins with molecular weights in the range of 120 to 200 give the best performance in describing the different properties of jet fuels. Of the compound types that they studied, these cycloparaffins were the only ones to show simultaneously the following properties [13]:

- o high heating value by volume
- o satisfactory heating value by weight
- o excellent thermal stability
- o very low freezing point
- o low volatility, high flash point
- o acceptable low-temperature viscosity
- o acceptable flame characteristics (smoke point, etc.)

"No other hydrocarbons in the jet-boiling-range have all of these properties [13]." Analyses of the four ITSL jet-boiling-range products at PETC (Table 4) confirm that the predominant compounds classes are indeed 1-, 2-, and 3-ring cycloparaffins, and the molecular weights (Table 1) are slightly below 200. Analysis of the Wyodak Light ITSL Syncrude by LVHRMS required 31 compound types in the range C_5 - C_{21} to account for the sample, while the same analysis of the Wyodak light ITSL hydrotreated product required only 13 compound types in the range C_6 to C_{16} to account for the sample [41]. Thus, hydrotreating this syncrude resulted in a less complex sample. Part of this loss in diversity can be accounted for by the fact that a certain distillate range was selected for the product, but in part, the diversity is lower because of heteroatom removal. Conceivably, a processing mode could be developed that would result in a product consisting of only a few compounds. The GPGP tar oil and overhead both fall in the molecular weight range of jet products, but only the overhead has the right boiling range. The GPGP overhead, however, has a high heteroatom content (37.81% C_6 - C_{12} hydroxybenzenes), as measured by LVHRMS (Table 5). The phenolic oxygen in the tar bottoms is less than half of that in the overhead (Table 2).

The GPGP tar oil, as well as the 350°C overhead and 350°C+ bottoms, is clearly very different (see Tables 1 and 2) from the coal liquefaction syncrudes evaluated by Sullivan. The twelve predominant compound types (from LVHRMS) found in the tar, the distillate overheads, and the bottoms are given in Table 5. The tar oil contains 33% of C_6 - C_{12} hydroxybenzenes, and the overheads contain almost 38%. The bottoms contain no large quantities of any compound types. The differences are most obvious in the NMR data (Table 2). Aromatic hydrogen and aromatic carbon are significantly higher in the GPGP tar oil samples. The weight percent oxygen as phenols (Table 2) is also higher in the GPGP samples. Surprisingly, the hydrotreated GPGP 350°C+ bottoms have properties very similar to the

Wyodak heavy ITSL syncrude. Presumably, this material could be further processed to produce a jet-fuel fraction that would have properties similar to the jet fraction produced by hydrotreating the Wyodak heavy ITSL syncrude. Similarly, the overheads could be hydrotreated to produce a jet-fuel-like distillate product. However, the oxygen content of the overhead fraction would require efficient heteroatom removal because oxygen functionalities have been implicated in problems with stability upon storage.

Correlations developed for narrow-boiling-range coal liquids [41] were successfully applied to the GPGP tar oil products as well as to the syncrudes and jet-boiling-range products. The results are reported in Table 6. The Illinois ITSL hydrocracked product gave the largest error when correlations were used to estimate molecular weight (15.93%) and refractive index (4.26%). An error of 7.8% resulted from estimation of the molecular weight of the tar oil, and an error of 1.32% resulted from estimation of the refractive index of the Wyodak heavy ITSL hydrotreated product. It is unclear why the hydrocracked product properties are difficult to estimate, but if this product is eliminated from the set, the average error in the estimated molecular weight is 2.37%, and the average error in the estimated refractive index is 0.49%. Khan recently reported successful applications of correlations based on refractive index to other liquids produced by coal pyrolysis [44].

Finally, bench-scale experiments conducted by Amoco have provided the basis for a process plan, established pilot-plant conditions, and produced small amounts of JP-8, JP-8X, and JP-4 jet fuels from GPGP tar oil [27]. With clay treatment and antioxidant additives, the JP-4 product was expected to meet all specifications except heating value, and the JP-8 and JP-8X were expected to meet all specifications except flash point. Two barrels of JP-8 jet fuel were jointly produced by Amoco and Lummus for evaluation by the Air Force.

CONCLUSIONS

Jet fuels can be prepared from a wide range of coal liquids produced in single-stage and two-stage liquefaction processes, as well as from by-product streams of gasification processes. The high aromaticity of coal, the very property that makes it an excellent candidate as a feedstock for high-density fuels, exacts a heavy penalty, however, in hydrogen consumption. The high heteroatom content not only consumes large amounts of hydrogen to produce mostly NH_3 , H_2S , and H_2O , but the remaining nitrogen tends to poison catalysts, and the nitrogen in jet fuel is blamed for gum formation. Oxygen compounds have been implicated in oxidative coupling reactions resulting in degradation of fuels upon storage.

In the future, with the decline in production of high-quality crudes, refiners will be pressed to process lower quality petroleum crudes. At some point then, production of jet fuels from coal will become an attractive and viable alternative. In the near term, there is still time to perform the requisite research yet remaining.

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DISCLAIMER

Reference in this paper to any specific commercial product, process, or service is to facilitate understanding and does not necessarily imply its endorsement or favoring by the United States Department of Energy.

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Table 1. Inspection Properties of Coal-Derived Jet-Boiling-Range Products, Syncrudes, and GPCP Tar Oil, Overhead, and Bottoms.

Sample	Boiling Range OF, 5-95%	T _b mid, OF	MM	RI	Specific Gravity	Density
Illinois ITSL Hydrotreated	302-561	462	185	1.4741	0.8750	0.8742
Illinois ITSL Hydrocracked	261-545	403	192	1.4600	0.8504	0.8497
Wyodak Heavy ITSL Hydrotreated	302-566	454	187	1.4679	0.8596	0.8589
Wyodak Light ITSL Hydrotreated	359-567	484	188	1.4772	0.8840	0.8832
Illinois ITSL Syncrude	212-731	546	201	1.5314	0.9513	0.9505
Wyodak Heavy ITSL Syncrude	347-850	652	229	1.5733	1.0074	1.0065
Wyodak Light ITSL Syncrude	331-713	575	205	1.5360	0.9596	0.9588
Great Plains Tar Oil	287-873	545	187	1.5700	ND	1.0193
GPCP Tar Overhead	274-665	472	155	1.5471	ND	0.9674
GPCP Tar Bottoms	652-967	776	355	ND	ND	1.0990
GPCP Tar Bottoms Hydrotreated	517-956	738	ND	ND	ND	ND

ND means not determined.

Table 2. NMR and IR Characterization of Coal-Derived Product

Sample	H-Aromatic Fraction	H _a	H _g	H _y	C Aromatic	wt% Oxygen as Phenols
Illinois ITSL Hydrotreated	0.02	0.03	0.69	0.26	0.04	ND
Illinois ITSL Hydrocracked	0.01	0.02	0.61	0.36	0.00	ND
Wyodak Heavy ITSL Hydrotreated	0.01	0.01	0.69	0.29	0.03	ND
Wyodak Light ITSL Hydrotreated	0.01	0.01	0.70	0.28	0.02	ND
Illinois ITSL Syncrude	0.14	0.16	0.53	0.17	0.38	0.1
Wyodak Heavy ITSL Syncrude	0.19	0.21	0.47	0.13	0.49	0.1
Wyodak Light ITSL Syncrude	0.14	0.15	0.53	0.18	0.35	0.1
Great Plains Tar Oil	0.24	0.32	0.35	0.09	0.69	2.4
GPCP Tar Overhead	0.26	0.36	0.30	0.08	0.64	3.2
GPCP Tar Bottoms	0.22	0.22	0.45	0.11	0.66	1.5
GPCP Tar Bottoms Hydrotreated	0.15	0.23	0.48	0.14	0.49	ND

ND means not determined.

Table 3. Properties of Jet Fuel Products

Sample	Illinois ITSL	Hydrocracked ^a	Illinois ITSL	Wyodak Heavy ITSL	Hydrocracked ^b	Wyodak Light ITSL	Hydrocracked ^c	Jet A ^d	High-Density ^e Fuel
Gravity, API	29	34	21	32	28	17	37 Min.	35 Min.	
Smoke Point, mm	19	21	21	21	17	17	20 Max.		
Freeze Point, °F	<-94	<-94	<-94	<-94	<-94	<-94	-40 Max.	-47 Max.	
Flash Point, °F	128	107	107	107	107	107	100 Min.	122 Min.	
Paraffins, LV %	1	2	7	7	5	5	0-10	0-10	
Naphthenes, LV %	91	96	82	82	86	86	70-90	70-90	
Aromatics, LV %	8	2	11	11	9	9	10-30	10-30	
Viscosity at -40°F, cSt	10.2	6.2					20 Max. 8 Max.	12 Max.	

^aReference 9; ^bReference 12; ^cReference 10; ^dReference 13; and ^eReference 42.

Table 4. Analysis of Jet-Boiling-Range Products by Mass Spectrometry

Compound Classes, Percent	Illinois ITSL Hydrocracked	Illinois ITSL Hydrocracked	Wyodak Heavy ITSL Hydrocracked	Wyodak Light ITSL Hydrocracked
Paraffins	4.16	2.59	8.26	5.95
Monocycloparaffins	20.54	53.29	39.44	35.88
Dicycloparaffins	53.23	27.64	30.45	33.83
Tricycloparaffins	12.92	11.88	13.27	15.80
Benzenes	6.45	4.33	3.99	5.21
Naphthalenes	0.31	0.14	0.23	2.76
Indans	2.39	0.13	4.37	0.53

NOTE: These analyses were obtained at low resolution with an ionizing voltage of 70 eV. The ASTM D2789 type analysis was used to calculate the compound classes.

Table 5. Analysis of Great Plains Tar Oil, 350°C Overheads, and 350°C+ Bottoms by LVHRMS
(Twelve Major Constituents)

Tar Oil	Overheads <350°C	Bottoms >350°C
33.00% C ₆ -C ₁₂ hydroxybenzenes	37.81% C ₆ -C ₁₂ hydroxybenzenes	7.05% C ₅ -C ₉ diolefins/cycloalkenes
11.71% C ₁₀ -C ₁₈ naphthalenes	14.72% C ₁₀ -C ₁₆ naphthalenes	6.98% C ₁₆ -C ₂₂ pyrenes
8.81% C ₆ -C ₁₅ benzenes	10.15% C ₆ -C ₁₅ benzenes	5.74% C ₁₄ -C ₂₁ phenanthrenes
4.78% C ₈ -C ₁₅ indans/tetralins	4.00% C ₅ -C ₁₀ pyridines	5.68% C ₅ -C ₉ olefins/cycloalkanes
3.70% C ₅ -C ₁₀ pyridines	3.98% C ₉ -C ₁₄ indans/tetralins	4.83% C ₁₃ -C ₂₀ hydroxyace- naphthalenes/hydroxyfluorenes
3.41% C ₈ -C ₁₄ hydroxyindenes	3.69% C ₈ -C ₁₄ hydroxyindenes	4.56% C ₁₄ -C ₂₀ hydroxyphenanthrenes
3.33% C ₁₀ -C ₁₇ hydroxynaphthalenes	3.03% C ₁₀ -C ₁₅ hydroxynaphthalenes	4.31% C ₁₆ -C ₂₂ hydroxypyrenes
3.32% C ₉ -C ₁₄ indenes	3.53% C ₉ -C ₁₄ indenes	4.40% C ₆ -C ₁₁ benzenes
2.68% C ₁₄ -C ₂₀ phenanthrenes	2.10% C ₅ -C ₉ diolefins/cycloalkenes	3.50% C ₁₂ -C ₁₈ hydroxybenzofurans/ dihydroxyfluorenes
2.33% C ₆ -C ₁₀ diolefins/cycloalkanes	1.80% C ₁₂ -C ₁₇ acenaphthylenes/ fluorenes	2.97% C ₁₀ -C ₁₅ naphthalenes
2.32% C ₅ -C ₉ olefins/cycloalkenes	1.64% C ₈ -C ₁₂ hydroxyindans/ hydroxytetralins	2.97% C ₁₈ -C ₂₄ chrysenes
2.20% C ₁₂ -C ₁₈ acenaphthylenes/ fluorenes	1.61% C ₁₄ -C ₁₈ phenanthrenes	2.85% C ₁₅ -C ₂₂ cyclopenta[def] phenanthrene/dihydropyrene

LVHRMS data taken from reference 40.

Table 6. Test of Fit to Existing Correlations Between Refractive Index, Molecular Weight, and Density

Sample	Refractive Index, n_D			Molecular Weight, M_w		
	Experimental	Calculated	% Error	Experimental	Calculated	% Error
Illinois ITSL Hydrotreated	1.4741	1.4625	0.79	185	182	1.80
Illinois ITSL Hydrocracked	1.4600	1.3978	4.26	192	161	15.93
Wyodak Heavy ITSL Hydrotreated	1.4679	1.4486	1.32	187	184	1.36
Wyodak Light ITSL Hydrotreated	1.4772	1.4784	0.08	188	189	0.51
Illinois ITSL Syncrude	1.5314	1.5168	0.96	201	198	1.61
Wyodak Heavy ITSL Syncrude	1.5733	1.5814	0.52	229	234	2.00
Wyodak Light ITSL Syncrude	1.5360	1.5381	0.14	205	210	2.21
Great Plains Tar Oil Feed	1.5700	1.5676	0.15	187	172	7.79
Great Plains Overhead	1.5471	1.5466	0.03	155	158	1.67

^aCalculated using Equations 1 and 2 of reference 41.

^bCalculated using Equation 5 of reference 41.